Nanotechnology Working Group

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Mission Statement

The National Cancer Institute (NCI) Cancer Biomedical Informatics Grid (caBIG®) Nanotechnology Working Group was established in 2008 for researchers with a specific interest in informatics and computational approaches to nanotechnology, with a particular emphasis on nanomedicine. The goal of this working group is to demonstrate the scientific potential of federating nanotechnology databases through pilot projects aimed at integrated semantic search and retrieval of nanomedicine and nanotoxicology datasets that are applicable across nanoscience. The caBIG® Nanotechnology Working Group (caBIG® Nano WG) comprises over 20 active participants from academia, government and industry with diverse interests.

Objectives

Long-term objectives

This Working Group is motivated by two high-priority nanomedicine informatics applications:

- The rational design of nanomaterials customized for use in nanomedicine.
- The development of robust structure-activity relationships to predict nanomaterial toxicity and to tailor this toxicity for therapeutic applications and/or to reduce hazards to health, safety and the environment.

These applications will be enabled by broad computational capability applied to nanotechnology research. The development of such capability has led to the following long-term objectives for the caBIG® Nano WG:

- To demonstrate a federated system of interoperable nanotechnology databases in the context of existing datasets and scientifically-relevant applications and user scenarios for nanotechnology.
- To develop a framework for uniform and comprehensive data curation and annotation while ensuring that data reliability and reproducibility is evaluated by those most familiar with both the data and the methods used to produce it.
- To establish a common framework for describing and accessing nanotechnology data using common data elements.
- To encourage the development of effective data mining standards and tools that are particularly suited for nanomaterial safety assessment, safe-by -design approaches, establishing nanotoxicology structure-activity relationships and nanomaterials characterization databases used for accompanying these objectives.
- To enable nanomedicine data search, sharing, and analysis through ontology development. One project directly related to this goal is the NanoParticle Ontology: http://nano-ontology.org.
- To facilitate nanomedicine and nanotoxicology data sharing and database interoperability through the development of standardized spreadsheet-based formats for nanotechnology datasets. One project directly derived from this goal is the nano-TAB standard for data submission: http://is.gd/foSKV.
- To encourage adoption and use of a shared informatics infrastructure by the nanotechnology and broader communities.

Short-term goals

To realize the long-term objectives outlined above, the caBIG® Nano WG has established several short-term goals with 6-12 month timeframes.
Defining basic nanomaterial characterizations. Careful physical, structural, and chemical characterizations are essential ingredients for nanomedicine informatics applications. While the fields of structural biology, genome sequencing, chemical synthesis, microarray analysis, etc. have defined basic assays for their respective technologies, the field of nanomedicine lacks a set of well-defined and "minimal" characterization methods for nanomaterials. There is an urgent need in the field to:

- Identify and describe the common types of nanomaterial characterizations, leveraging existing work by IANH, ASTM, ISO, and other organizations.
- Draft a standard for the minimal set of characterizations needed for nanomedicine informatics activities. The Working Group currently has broad representation from a variety of relevant agencies to undertake this task in a collaborative and inclusive manner.

Completed: See Nanocharacterization Library

Standardizing nanomaterial characterization protocols. Several Working Group members have noted that standard characterizations discussed above are only useful if the protocols for these characterizations are themselves standardized and reproducible. Furthermore, evidence from inter-laboratory studies by ASTM and IANH suggests that there is significant variability in results from existing "standard" protocols, suggesting that current mechanisms for protocol communication are ineffective. This nanotechnology problem is currently under investigation by ASTM and ISO groups. The Working Group assists in this effort by:

- Collecting standard methodologies related to the characterization activities described above.
- Providing a forum with a diverse group of participants for discussing the best mechanisms for sharing nanotechnology characterization protocols.
- Augmenting data with computational data.

On hold

Defining standards for nanomedicine data sharing and exchange. Currently, access to relevant data is a major barrier to the realization of the nanomedical goals of rational nanomaterial design and toxicity prediction. While a few detailed datasets exist for nanomaterial toxicity (ONAMI), and nanomaterial-cellular interactions (Shaw et al.) most of the necessary data is dispersed across a wide array of nanotechnology data resources. Therefore, it is essential to implement an infrastructure to ensure that these data can be shared among researchers and data resources. To develop this (federated) data sharing infrastructure, the Working Group has undertaken development of the nano-TAB spreadsheet form, based on the ISA-TAB framework, to facilitate submission of data by experimental researchers. The nano-TAB effort is translating the great success of MAGE-TAB microarray and similar formats for enabling data sharing in other communities. The nano-TAB project is actively growing and under development as an ASTM standard (WK28974 at http://is.gd/foSKV)

Completed. Ongoing development based on community requirements and feedack: See nano-TAB Specification

Providing vocabulary and semantic support to the nanomedicine community. Data generated from nanotechnology research are so diverse and large in volume that it is difficult to share and efficiently use them without informatics tools. In particular, ontologies that provide a unifying knowledge framework for annotating the data are required to facilitate the semantic integration, knowledge-based searching, unambiguous interpretation, mining and inferencing of the data using informatics methods. The caBIG® Nano WG supports the continuing development and application the of NanoParticle Ontology (NPO), which is developed within the framework of the Basic Formal Ontology (BFO), and implemented in the Ontology Web Language (OWL) using well-defined ontology design principles. The NPO was developed to represent knowledge underlying the preparation, chemical composition and characterization of nanomaterials involved in research.

Ongoing development based on community requirements and feedback: More information can be found at http://nano-ontology.org.

Schedule

Click Here to see the spreadsheet listing speakers and milestones for Aug 2011 - Dec 2011.

Participation and Communication

The Nanotechnology Working Group is a working group of the caBIG® ICR Workspace and is expected to work closely with the caBIG community, including other Workspaces and ICR Working groups.
Participation

Nanotechnology working group calls are open to anyone interested in participating in and contributing to the working group discussions and activities.

Meetings

Nano WG meetings will take place on every Thursday at 1 pm ET.

- Teleconference call-in: 800-593-0616, passcode: 77412
- Web conference is: http://cbiit.adobeconnect.com/nanowg

Group Communications
Group communications will be managed through the Working Group wiki site (here) and the Nano-Standards listserv.

Teleconference Materials

*The meeting **Date** is hyperlinked to the notes and hyperlinks in the **Executive Summary** are for specific presentations*

Date	Executive Summary	Sub Group Updates